



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 11:09 AM GMT

PDB ID : 3O6X
Title : Crystal Structure of the type III Glutamine Synthetase from *Bacteroides fragilis*
Authors : van Rooyen, J.M.; Belrhali, H.; Abratt, V.R.; Sewell, B.T.
Deposited on : 2010-07-29
Resolution : 3.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

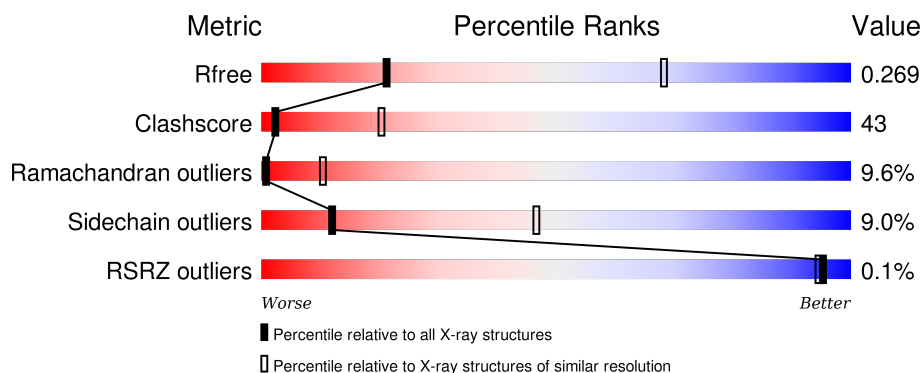
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	729	
1	B	729	
1	C	729	
1	D	729	
1	E	729	

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Mol	Chain	Length	Quality of chain
1	F	729	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ADP	B	4001	-	-	-	X
4	ADP	E	4001	-	-	-	X
5	CL	A	6001	-	-	X	-
5	CL	A	730	-	-	X	-
5	CL	B	5001	-	-	-	X
5	CL	B	6001	-	-	X	-
5	CL	C	5001	-	-	-	X
5	CL	C	6001	-	-	X	-
5	CL	D	6001	-	-	X	-
5	CL	E	6001	-	-	X	-
5	CL	F	6001	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 30996 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Glutamine synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	638	Total	C	N	O	S	250	0	0
			5120	3253	889	948	30			
1	B	638	Total	C	N	O	S	250	0	0
			5120	3253	889	948	30			
1	C	638	Total	C	N	O	S	250	0	0
			5120	3253	889	948	30			
1	D	638	Total	C	N	O	S	250	0	0
			5120	3253	889	948	30			
1	E	638	Total	C	N	O	S	250	0	0
			5120	3253	889	948	30			
1	F	638	Total	C	N	O	S	250	0	0
			5120	3253	889	948	30			

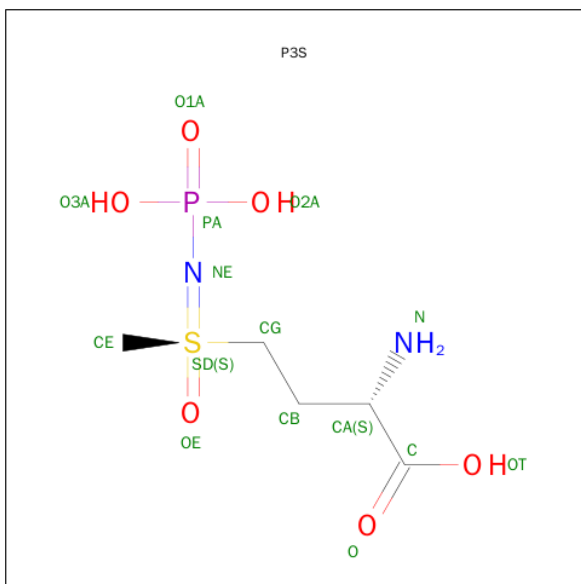
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	152	GLY	VAL	CONFLICT	UNP Q5LGP1
A	531	LEU	PRO	CONFLICT	UNP Q5LGP1
B	152	GLY	VAL	CONFLICT	UNP Q5LGP1
B	531	LEU	PRO	CONFLICT	UNP Q5LGP1
C	152	GLY	VAL	CONFLICT	UNP Q5LGP1
C	531	LEU	PRO	CONFLICT	UNP Q5LGP1
D	152	GLY	VAL	CONFLICT	UNP Q5LGP1
D	531	LEU	PRO	CONFLICT	UNP Q5LGP1
E	152	GLY	VAL	CONFLICT	UNP Q5LGP1
E	531	LEU	PRO	CONFLICT	UNP Q5LGP1
F	152	GLY	VAL	CONFLICT	UNP Q5LGP1
F	531	LEU	PRO	CONFLICT	UNP Q5LGP1

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	2	Total 2 Mg 2	0	0
2	E	2	Total 2 Mg 2	0	0
2	B	2	Total 2 Mg 2	0	0
2	C	2	Total 2 Mg 2	0	0
2	A	2	Total 2 Mg 2	0	0
2	F	2	Total 2 Mg 2	0	0

- Molecule 3 is L-METHIONINE-S-SULFOXIMINE PHOSPHATE (three-letter code: P3S) (formula: $C_5H_{13}N_2O_6PS$).



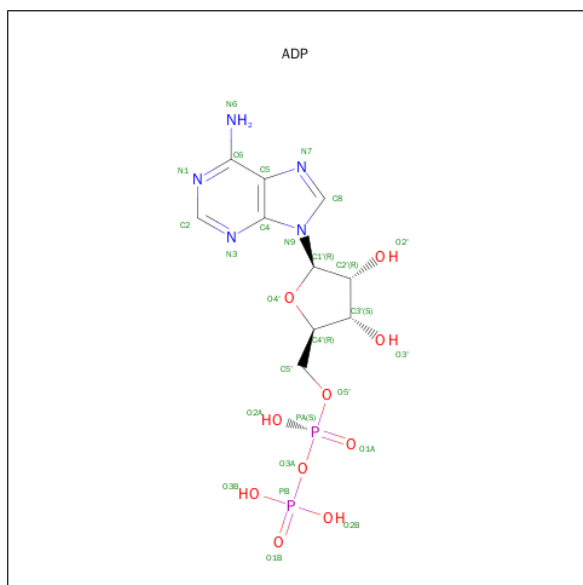
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total 15 C 5 N 2 O 6 P 1 S 1	0	0
3	B	1	Total 15 C 5 N 2 O 6 P 1 S 1	0	0
3	C	1	Total 15 C 5 N 2 O 6 P 1 S 1	0	0
3	D	1	Total 15 C 5 N 2 O 6 P 1 S 1	0	0
3	E	1	Total 15 C 5 N 2 O 6 P 1 S 1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	F	1	Total	C	N	O	P	S	
			15	5	2	6	1	1	
								0	0

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P		
			27	10	5	10	2	0	0
4	B	1	Total	C	N	O	P		
			27	10	5	10	2	0	0
4	C	1	Total	C	N	O	P		
			27	10	5	10	2	0	0
4	D	1	Total	C	N	O	P		
			27	10	5	10	2	0	0
4	E	1	Total	C	N	O	P		
			27	10	5	10	2	0	0
4	F	1	Total	C	N	O	P		
			27	10	5	10	2	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	2	Total 2 Cl	0	0
5	E	2	Total 2 Cl	0	0

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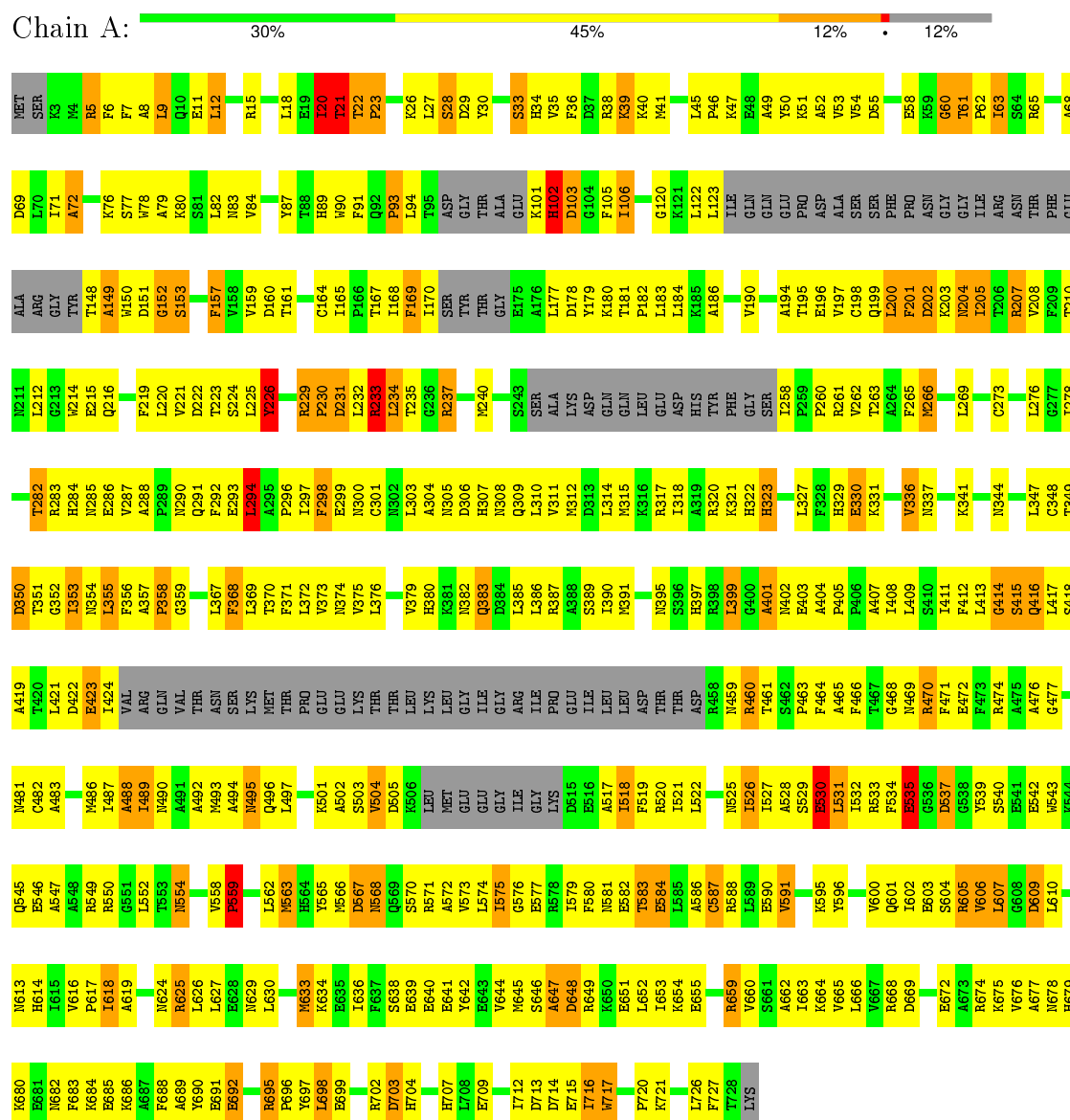
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total 2	Cl 2	0	0
5	C	2	Total 2	Cl 2	0	0
5	A	3	Total 3	Cl 3	0	0
5	F	1	Total 1	Cl 1	0	0

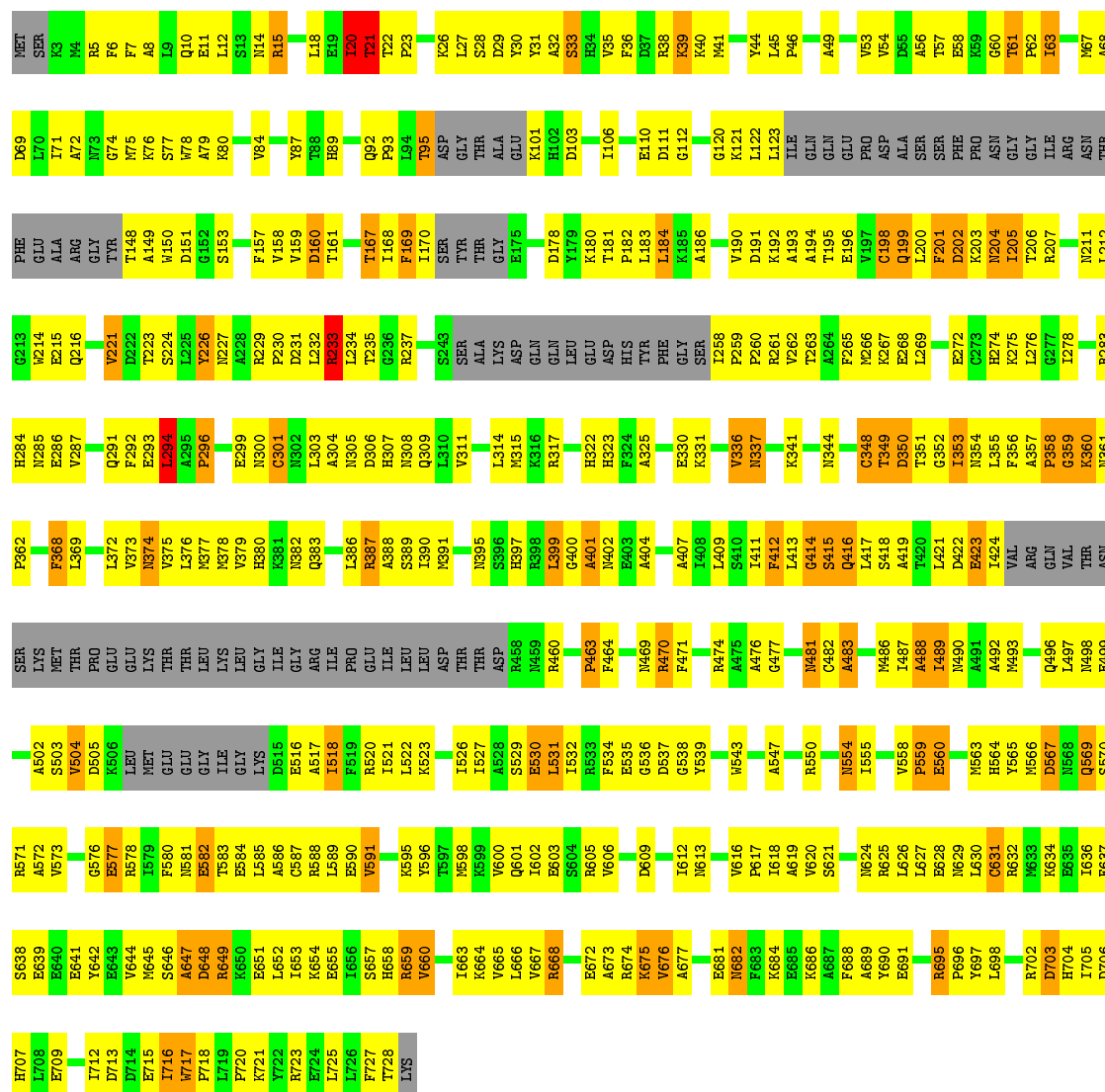
3 Residue-property plots

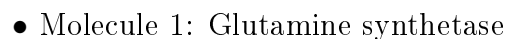
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

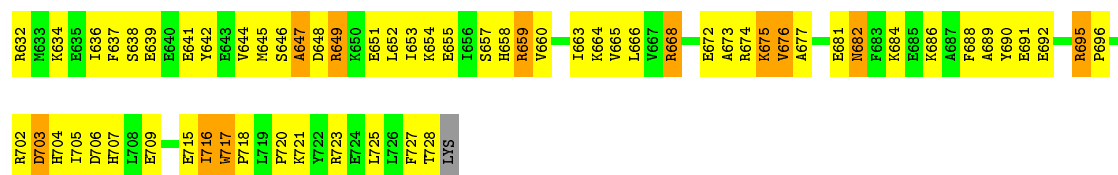
• Molecule 1: Glutamine synthetase



Chain B:  33% 45% 10% 12%

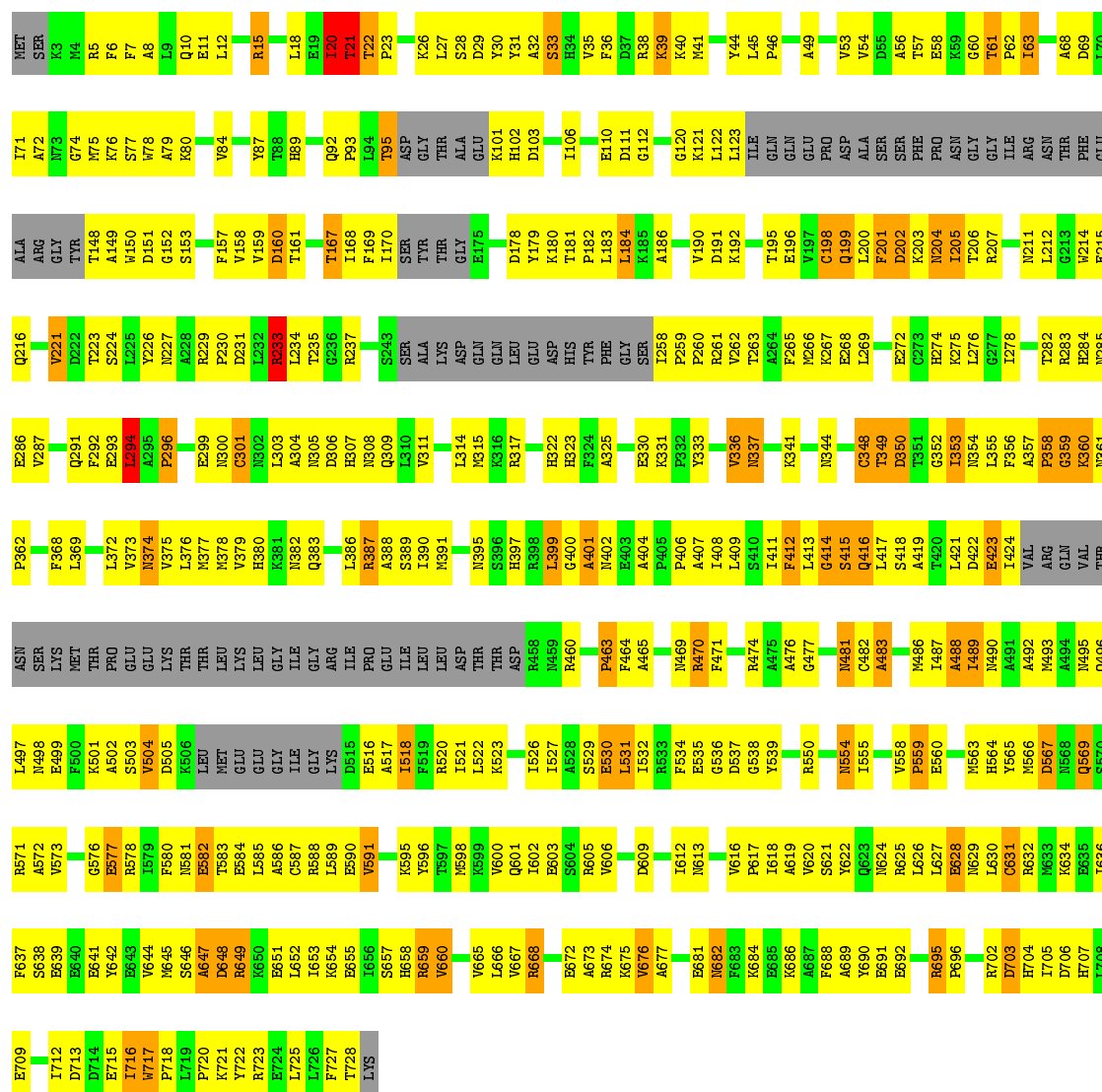






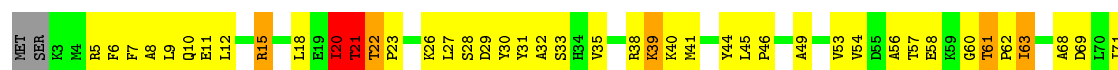
• Molecule 1: Glutamine synthetase

Chain E: 33% 45% 9% 12%



• Molecule 1: Glutamine synthetase

Chain F: 34% 43% 10% 12%



E715	E716	E717	F718	L719	F720	D721	F722	R723	E724	L725	L726	F727	T728	LYS	Y642	E643	M644	M645	S646	A647	D648	R649	K650	E651	L652	I653	K654	E655	I656	S657	R658	R659	V660	I663	K664	V665	L666	V667	R668	E672	A673	R674	K675	V676	A677	E681	N682	K686	A687	F688	A689	Y690	E691	E692	R695	P696	R702	D703	H704	I705	D706	H707	L708	E709	I712	D713	D714
G576	G577	R578	L579	F580	N581	E582	T583	L584	L585	A586	C587	R588	L589	E590	V591	K595	F596	T597	M598	R599	V600	Q601	I602	E603	S604	R605	V606	D609	N613	V616	P617	L618	A619	Y622	Q623	N624	R625	L626	L627	N629	L630	C631	R632	L633	K634	E635	I636	F637	S638	E639	E640	E641															
E499	F500	K501	A502	S503	V504	D505	K506	LEU	MET	L585	A586	C587	R588	L589	E590	V591	K595	F596	T597	M598	R599	V600	Q601	I602	E603	S604	R605	V606	D609	N613	V616	P617	L618	A619	Y622	Q623	N624	R625	L626	L627	N629	L630	C631	R632	L633	K634	E635	I636	F637	S638	E639	E640	E641														
ASN	SER	LYS	MET	THR	PRO	GLU	GLU	LYS	THR	THR	LEU	LYS	LEU	GLY	ILE	LYS	GLY	ARG	ILE	PRO	GLU	ILE	ASP	THR	THR	ASP	R458	R459	R460	P463	F464	N469	R470	F471	R474	A475	A476	G477	M481	C482	A483	M486	I487	A488	I489	M490	A491	A492	M493	Q496	L497	M498															
ASN	SER	LYS	MET	THR	PRO	GLU	GLU	LYS	THR	THR	LEU	LYS	LEU	GLY	ILE	LYS	GLY	ARG	ILE	PRO	GLU	ILE	ASP	THR	THR	ASP	R458	R459	R460	P463	F464	N469	R470	F471	R474	A475	A476	G477	M481	C482	A483	M486	I487	A488	I489	M490	A491	A492	M493	Q496	L497	M498															
N361	P362	F368	L369	L372	N373	N374	V375	L376	K377	K378	V379	H380	K381	Q383	L386	R387	A388	S389	I390	K391	N395	S396	N397	R398	L399	G400	A401	E403	A404	A407	F408	L409	S410	I411	F412	L413	G414	S415	Q416	L417	S418	A419	T420	L421	D422	E423	I424	VAL	ARG	GLN	VAL	THR															
N361	P362	F368	L369	L372	N373	N374	V375	L376	K377	K378	V379	H380	K381	Q383	L386	R387	A388	S389	I390	K391	N395	S396	N397	R398	L399	G400	A401	E403	A404	A407	F408	L409	S410	I411	F412	L413	G414	S415	Q416	L417	S418	A419	T420	L421	D422	E423	I424	VAL	ARG	GLN	VAL	THR															
H284	N285	E286	V287	N290	Q291	F292	E293	L294	A295	P296	E299	N300	C301	N302	L303	A304	N305	D306	H307	N308	I309	Q309	ALA	V311	L314	N315	K316	R317	H322	H323	F324	A325	E330	K331	V336	N337	K341	N344	C348	T349	D350	T351	G352	L353	N354	L355	F356	A357	P358	G359	K360																
H284	N285	E286	V287	N290	Q291	F292	E293	L294	A295	P296	E299	N300	C301	N302	L303	A304	N305	D306	H307	N308	I309	Q309	ALA	V311	L314	N315	K316	R317	H322	H323	F324	A325	E330	K331	V336	N337	K341	N344	C348	T349	D350	T351	G352	L353	N354	L355	F356	A357	P358	G359	K360																
Q216	F219	L220	D221	D222	T223	S224	L225	Y226	D227	A228	R229	P230	D231	T232	L233	L234	T235	G236	R237	S243	SER	ALA	LYS	ASP	GLN	GLN	LEU	GLU	ASP	HIS	TYR	PHE	GLY	T258	P259	R261	T262	T263	A264	F265	M266	K267	E268	D202	L269	E272	C273	K274	K275	L276	G277	I278	T282	R283													
Q216	F219	L220	D221	D222	T223	S224	L225	Y226	D227	A228	R229	P230	D231	T232	L233	L234	T235	G236	R237	S243	SER	ALA	LYS	ASP	GLN	GLN	LEU	GLU	ASP	HIS	TYR	PHE	GLY	T258	P259	R261	T262	T263	A264	F265	M266	K267	E268	D202	L269	E272	C273	K274	K275	L276	G277	I278	T282	R283													
ARG	GLY	TYR	T148	A149	W150	D151	G152	S153	F157	V158	V159	D160	T161	T167	I168	F169	I170	SER	GLY	THR	GLY	ALA	LYS	D178	Y179	K180	T181	P182	L183	L184	K185	A186	V190	D191	K192	A193	T195	T262	E196	Y197	C198	Q199	L200	SER	F201	PHE	PRO	ASN	GLY	ILE	ARG	ASN	THR	PHE	GLU	ALA											
ARG	GLY	TYR	T148	A149	W150	D151	G152	S153	F157	V158	V159	D160	T161	T167	I168	F169	I170	SER	GLY	THR	GLY	ALA	LYS	D178	Y179	K180	T181	P182	L183	L184	K185	A186	V190	D191	K192	A193	T195	T262	E196	Y197	C198	Q199	L200	SER	F201	PHE	PRO	ASN	GLY	ILE	ARG	ASN	THR	PHE	GLU	ALA											

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	198.25Å 203.96Å 234.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.87 – 3.50 62.87 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (62.87-3.50) 100.0 (62.87-3.50)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	0.21	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.94 (at 3.49Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.239 , 0.269 0.239 , 0.269	Depositor DCC
R_{free} test set	3016 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	52.8	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 70.8	EDS
Estimated twinning fraction	0.014 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 60072 reflections	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	30996	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: P3S, MG, ADP, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.47	0/5223	0.68	1/7048 (0.0%)
1	B	0.43	0/5223	0.63	1/7048 (0.0%)
1	C	0.43	0/5223	0.63	1/7048 (0.0%)
1	D	0.43	0/5223	0.63	1/7048 (0.0%)
1	E	0.44	0/5223	0.63	1/7048 (0.0%)
1	F	0.43	0/5223	0.63	1/7048 (0.0%)
All	All	0.44	0/31338	0.64	6/42288 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	233	ARG	N-CA-C	-5.70	95.60	111.00
1	B	233	ARG	N-CA-C	-5.68	95.67	111.00
1	E	233	ARG	N-CA-C	-5.59	95.91	111.00
1	D	233	ARG	N-CA-C	-5.57	95.97	111.00
1	F	233	ARG	N-CA-C	-5.55	96.02	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	226	TYR	Sidechain
1	B	226	TYR	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5120	0	5090	481	0
1	B	5120	0	5090	415	1
1	C	5120	0	5090	402	0
1	D	5120	0	5090	406	0
1	E	5120	0	5090	415	0
1	F	5120	0	5090	409	1
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	15	0	10	1	0
3	B	15	0	10	0	0
3	C	15	0	10	0	0
3	D	15	0	10	0	0
3	E	15	0	10	0	0
3	F	15	0	10	0	0
4	A	27	0	12	4	0
4	B	27	0	12	2	0
4	C	27	0	12	2	0
4	D	27	0	12	2	0
4	E	27	0	12	2	0
4	F	27	0	12	2	0
5	A	3	0	0	5	0
5	B	2	0	0	4	0
5	C	2	0	0	4	0
5	D	2	0	0	4	0
5	E	2	0	0	4	0
5	F	1	0	0	3	0
All	All	30996	0	30672	2496	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 43.

The worst 5 of 2496 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:ILE:HD13	1:A:170:ILE:HD13	1.47	0.97
1:B:229:ARG:HD3	1:B:720:PRO:HD2	1.47	0.97
1:C:20:ILE:HG12	1:C:21:THR:H	1.31	0.96
1:F:229:ARG:HD3	1:F:720:PRO:HD2	1.46	0.96
1:F:20:ILE:HG12	1:F:21:THR:H	1.29	0.96

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:651:GLU:OE1	1:F:423:GLU:OE2[8_457]	2.18	0.02

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	624/729 (86%)	408 (65%)	148 (24%)	68 (11%)	0	8
1	B	624/729 (86%)	438 (70%)	128 (20%)	58 (9%)	1	11
1	C	624/729 (86%)	441 (71%)	124 (20%)	59 (10%)	1	10
1	D	624/729 (86%)	433 (69%)	132 (21%)	59 (10%)	1	10
1	E	624/729 (86%)	444 (71%)	121 (19%)	59 (10%)	1	10
1	F	624/729 (86%)	442 (71%)	124 (20%)	58 (9%)	1	11
All	All	3744/4374 (86%)	2606 (70%)	777 (21%)	361 (10%)	1	10

5 of 361 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	ILE
1	A	23	PRO
1	A	149	ALA
1	A	204	ASN
1	A	234	LEU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	554/631 (88%)	496 (90%)	58 (10%)	8	38
1	B	554/631 (88%)	506 (91%)	48 (9%)	13	48
1	C	554/631 (88%)	506 (91%)	48 (9%)	13	48
1	D	554/631 (88%)	505 (91%)	49 (9%)	12	48
1	E	554/631 (88%)	508 (92%)	46 (8%)	14	50
1	F	554/631 (88%)	505 (91%)	49 (9%)	12	48
All	All	3324/3786 (88%)	3026 (91%)	298 (9%)	12	46

5 of 298 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	387	ARG
1	D	184	LEU
1	F	350	ASP
1	C	481	ASN
1	C	676	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 99 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	678	ASN
1	D	382	ASN
1	F	481	ASN
1	C	707	HIS

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Mol	Chain	Res	Type
1	D	285	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 36 ligands modelled in this entry, 24 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	P3S	A	3001	2	10,14,14	3.44	4 (40%)	6,21,21	5.91	4 (66%)
4	ADP	A	4001	2	22,29,29	1.01	1 (4%)	27,45,45	2.58	9 (33%)
3	P3S	B	3001	2	10,14,14	3.45	4 (40%)	6,21,21	6.09	4 (66%)
4	ADP	B	4001	2	22,29,29	1.01	1 (4%)	27,45,45	2.59	9 (33%)
3	P3S	C	3001	2	10,14,14	3.44	4 (40%)	6,21,21	6.10	4 (66%)
4	ADP	C	4001	2	22,29,29	1.01	1 (4%)	27,45,45	2.58	9 (33%)
3	P3S	D	3001	2	10,14,14	3.43	4 (40%)	6,21,21	6.14	4 (66%)
4	ADP	D	4001	2	22,29,29	1.00	1 (4%)	27,45,45	2.60	9 (33%)
3	P3S	E	3001	2	10,14,14	3.44	4 (40%)	6,21,21	6.10	4 (66%)
4	ADP	E	4001	2	22,29,29	1.00	1 (4%)	27,45,45	2.58	9 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	P3S	F	3001	2	10,14,14	3.44	4 (40%)	6,21,21	6.16	4 (66%)
4	ADP	F	4001	2	22,29,29	1.00	1 (4%)	27,45,45	2.59	9 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	P3S	A	3001	2	-	0/5/16/16	0/0/0/0
4	ADP	A	4001	2	-	0/12/32/32	0/3/3/3
3	P3S	B	3001	2	-	0/5/16/16	0/0/0/0
4	ADP	B	4001	2	-	0/12/32/32	0/3/3/3
3	P3S	C	3001	2	-	0/5/16/16	0/0/0/0
4	ADP	C	4001	2	-	0/12/32/32	0/3/3/3
3	P3S	D	3001	2	-	0/5/16/16	0/0/0/0
4	ADP	D	4001	2	-	0/12/32/32	0/3/3/3
3	P3S	E	3001	2	-	0/5/16/16	0/0/0/0
4	ADP	E	4001	2	-	0/12/32/32	0/3/3/3
3	P3S	F	3001	2	-	0/5/16/16	0/0/0/0
4	ADP	F	4001	2	-	0/12/32/32	0/3/3/3

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	3001	P3S	PA-O3A	-2.88	1.48	1.54
3	A	3001	P3S	PA-O3A	-2.87	1.48	1.54
3	D	3001	P3S	PA-O3A	-2.86	1.48	1.54
3	E	3001	P3S	PA-O3A	-2.85	1.48	1.54
3	C	3001	P3S	PA-O3A	-2.85	1.48	1.54

The worst 5 of 78 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	3001	P3S	OE-SD-CG	-12.30	99.70	108.23
3	D	3001	P3S	OE-SD-CG	-12.29	99.70	108.23
3	C	3001	P3S	OE-SD-CG	-12.15	99.80	108.23
3	E	3001	P3S	OE-SD-CG	-12.14	99.81	108.23
3	B	3001	P3S	OE-SD-CG	-12.11	99.83	108.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3001	P3S	1	0
4	A	4001	ADP	4	0
4	B	4001	ADP	2	0
4	C	4001	ADP	2	0
4	D	4001	ADP	2	0
4	E	4001	ADP	2	0
4	F	4001	ADP	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	637/729 (87%)	-0.46	0 100 100	2, 25, 71, 127	51 (8%)
1	B	637/729 (87%)	-0.40	0 100 100	2, 33, 89, 150	51 (8%)
1	C	637/729 (87%)	-0.32	1 (0%) 95 93	2, 31, 85, 149	51 (8%)
1	D	637/729 (87%)	-0.39	0 100 100	2, 29, 79, 148	51 (8%)
1	E	637/729 (87%)	-0.45	0 100 100	2, 32, 82, 169	51 (8%)
1	F	637/729 (87%)	-0.36	1 (0%) 95 93	2, 31, 81, 129	51 (8%)
All	All	3822/4374 (87%)	-0.40	2 (0%) 95 94	2, 30, 82, 169	306 (8%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	200	LEU	3.6
1	C	549	ARG	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	CL	C	5001	1/1	0.99	0.26	3.16	1,1,1,1	0
5	CL	B	5001	1/1	0.95	0.25	2.51	1,1,1,1	0
4	ADP	E	4001	27/27	0.82	0.29	2.35	99,113,123,125	0
4	ADP	B	4001	27/27	0.80	0.32	2.25	102,116,127,128	0
4	ADP	A	4001	27/27	0.82	0.29	1.66	80,94,104,106	0
4	ADP	D	4001	27/27	0.81	0.33	1.55	93,107,117,118	0
4	ADP	F	4001	27/27	0.82	0.30	1.12	88,102,113,114	0
3	P3S	A	3001	15/15	0.83	0.33	1.06	118,128,135,138	0
3	P3S	F	3001	15/15	0.88	0.32	1.04	118,128,135,138	0
3	P3S	D	3001	15/15	0.85	0.28	0.95	118,128,135,138	0
5	CL	A	730	1/1	0.97	0.21	0.94	1,1,1,1	0
4	ADP	C	4001	27/27	0.82	0.25	0.89	99,113,124,125	0
3	P3S	E	3001	15/15	0.80	0.30	0.88	118,128,135,138	0
3	P3S	C	3001	15/15	0.79	0.25	0.55	118,128,135,138	0
5	CL	A	5001	1/1	0.97	0.18	0.30	1,1,1,1	0
3	P3S	B	3001	15/15	0.83	0.23	0.07	118,128,135,138	0
5	CL	D	5001	1/1	0.98	0.19	-0.00	1,1,1,1	0
5	CL	E	5001	1/1	0.96	0.15	-0.43	1,1,1,1	0
2	MG	D	2001	1/1	0.94	0.31	-	32,32,32,32	0
2	MG	C	1001	1/1	0.88	0.15	-	8,8,8,8	0
5	CL	F	6001	1/1	0.96	0.13	-	1,1,1,1	0
2	MG	E	1001	1/1	0.91	0.09	-	10,10,10,10	0
2	MG	E	2001	1/1	0.76	0.23	-	41,41,41,41	0
5	CL	E	6001	1/1	0.95	0.13	-	5,5,5,5	0
5	CL	C	6001	1/1	0.94	0.09	-	10,10,10,10	0
2	MG	F	1001	1/1	0.88	0.14	-	23,23,23,23	0
5	CL	B	6001	1/1	0.92	0.07	-	5,5,5,5	0
2	MG	D	1001	1/1	0.90	0.21	-	10,10,10,10	0
2	MG	B	1001	1/1	0.72	0.20	-	15,15,15,15	0
2	MG	A	1001	1/1	0.92	0.17	-	3,3,3,3	0
5	CL	D	6001	1/1	0.89	0.16	-	4,4,4,4	0
2	MG	B	2001	1/1	0.90	0.15	-	52,52,52,52	0
2	MG	F	2001	1/1	0.81	0.24	-	30,30,30,30	0
2	MG	A	2001	1/1	0.91	0.14	-	37,37,37,37	0
2	MG	C	2001	1/1	0.91	0.30	-	33,33,33,33	0
5	CL	A	6001	1/1	0.94	0.12	-	2,2,2,2	0

6.5 Other polymers ⓘ

There are no such residues in this entry.